BRIDGING THE GAP BETWEEN WELL-DEFINED AND INDUSTRIAL CATALYSTS VIA A MOLECULAR APPROACH

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Industrial processes, in particular large-scale ones, mostly rely on heterogeneous catalysts. The search for more sustainable processes and the changes in environmental policies impose the continuous development of improved catalyst performances and catalytic processes, as well as the exploration of alternative routes. However, due to their inherent complexity, heterogeneous catalysts are mostly developed empirically rather than through detailed structure – activity relationships as the nature of the active sites are rarely known.

In this context, our group has been interested in understanding and controlling chemistry on surfaces, with the ultimate goal to generate isolated metal sites with defined chemical environment.[1] This approach has been used to develop highly active and selective single-site catalysts that can overperform their homogeneous counterparts, but it can also provide useful information to understand and further develop industrial catalysts[2] or to study much more complex systems such as supported nanoparticles, where support effects, interfaces, alloying… remain complex to understand at the molecular level.

This lecture will be developed around these themes and will show that a careful characterization of surface sites on a molecular level is key to develop high performance catalysts and to bridge the gap between fundamental and applied catalysis.[3] We will also look at how NMR chemical shifts can be used as a very powerful descriptor of reactivity for molecular and supported single-site catalysts.[4]

References:

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